

A Characterization of Topological Insulators: Chern Numbers for a Ground State Multiplet

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We propose to use generic Chern numbers for a characterization of topological insulators. It is suitable for a numerical characterization of low dimensional quantum liquids where strong quantum fluctuations prevent from developing conventional orders. By twisting parameters of boundary conditions, the non-Abelian Chern number are defined for a few low lying states near the ground state in a finite system, which is a ground state multiplet with a possible (topological) degeneracy. We define the system as a topological insulator when energies of the multiplet are well separated from the above. Translational invariant twists up to a unitary equivalence are crucial to pick up only bulk properties without edge states. As a simple example, the setup is applied for a two-dimensional XXZ -spin system with an ising anisotropy where the ground state multiplet is composed of doubly almost degenerate states. It gives a vanishing Chern number due to a symmetry. Also Chern numbers for the generic fractional quantum Hall states are discussed shortly.

A crucial role of phases is one of intrinsic features of quantum mechanics and has a long history of investigation. Among them, those which have intrinsic geometric origins are now understood as geometrical phases[1]. Aharonov-Bohm effects and Dirac monopoles are typical and classic examples where the geometrical phases are fundamental. Geometrical features of gauge theories are another prototype[2]. Also a discovery of Berry's phases reveals that the geometric phases and the gauge structure are closely related and derived by restricting a physical Hilbert space[3, 4].

On the other hand, with an idea of order parameters, symmetry breaking is one of the most fundamental concepts in modern physics. Quite successfully, this standard setup can characterize most of ordered states and describe phase transitions and critical phenomena. However in low dimensional quantum systems, such as electrons with strong correlation and spins, quantum fluctuations prevent from developing conventional orders even at a zero temperature. In these systems, quantum phases of manybody ground states vary wildly in space and time, which destroy the standard orders.

Of course, the wild quantum phases are not random but obey some hidden restriction rules and reflect features of the quantum mechanical wave function. Some of them are well known today such as Marshall sign rules in the spin systems[5] and fractional statistics of quasi-particle (hole) wavefunctions in the fractional quantum Hall effect (FQH)[6]. String order parameters in the Hal-dane spin chains[7, 8, 9] and the quasi off-diagonal order in the FQH[10] are also discussed based on the feature. Generically quantum states with the characteristic geometric phases are considered to possess non-trivial topological orders[11].

Recently wide variety of interesting and physically important phenomena have been understood based on a concept of the topological order. Some of

them include quantum Hall effects[12, 13], solitons in polyacetylenes[14], adiabatic transports of charge and spins[15], itinerant magnetism and spintronics[16] and anomalous Hall conductances[17, 18, 19], polarizations in insulators[20], the two dimensional carbon sheets[21, 22], anisotropic superconductors[22, 23, 24], and string-net condensations[25]. They are under active studies.

A local phase of the manybody wave function is arbitrary but there is some correlation with the phases of its neighbors, which brings some gauge structures. In these view points, templates of such systems are quantum Hall states, especially integer quantum Hall (IQH) states. There are apparently different QH states with different quantized Hall conductances. However, any symmetries are not broken among the states but they are clearly different physical systems. These states are characterized by the quantized Hall conductances which have an intrinsic topological origin[12]. The topological origin of the Hall conductance is clear by the Chern number expression[13, 26, 27]. Based on the observation, we *propose to characterize the topological orders by the generic Chern numbers*[28]. The Chern numbers in topological ordered systems are kinds of order parameters in conventional ordered phases. In the same manner as the usual phase transition is characterized by a sudden change of order parameters, topological phase transitions are characterized by a discontinuous change of the Chern numbers.

To have a well defined Chern number, we need an existence of a generic gap[28]. *Topological insulators* are defined as physical systems with this generic energy gap. Then the Chern numbers are always integers and the topological phase transition is characterized by a discontinuous change of the Chern numbers which are always integers. This integral property of the Chern number implies a stability of the characterization against a small perturbation. However, as in the case of the edge states of

the quantum Hall effect[29] and Kennedy's triplet states in the Haldane spin chains[30], the topological ordered state are quite sensitive to a geometrical change of the physical system such as an existence of edges and boundaries. It contrasts with the conventional order where boundary conditions are always negligible in the thermodynamic limit. Therefore a translational invariance is fundamentally important to describe topological ordered states. On the other hand, in many cases, as far as physical observables are concerned, a topological order is hidden in a bulk and only reveals its physical significance near boundaries of the system.

Generically speaking, to define the Chern numbers C for a physical (many particle) wave function, ψ , we need to require the wave function to depend on multiple parameters, $x \in \mathcal{V}$, $\dim \mathcal{V} \geq 2$. Most common such parameters without disturbing bulk properties are multiple Aharonov-Bohm fluxes on a genus g Riemann surface. When the topological order is non-trivial, there can be inevitable topological degeneracies[11], such as a q^g -fold degeneracy of the FQH state with a filling factor $1/q$ on a torus[31, 32, 33]. The degeneracy of a generic ground state will be discussed later. Here we just point out that one has to consider non-Abelian gauge structures arising from it[4, 28]. This is crucial for a numerical concrete characterization of the topological insulators. Especially an explicit gauge fixing for the degenerate multiplet is required to perform calculations.[28].

Quantum Spin Systems as Topological Insulators : To describe a characterization of the topological order, let us consider a generic translational invariant spin-1/2 hamiltonian on a d -dimensional orthogonal lattice $H^P = H(h_\ell) = \sum_{\mathbf{m}} T^{\mathbf{m}} h_\ell((\mathbf{S}(\mathbf{r}_1), \mathbf{S}(\mathbf{r}_2), \dots) T^{\mathbf{m}^\dagger}$ where $T^{\mathbf{m}} = T_1^{m_1} \cdots T_d^{m_d}$, $\mathbf{m} = (m_1, \dots, m_d)$ and ${}^t \mathbf{S}(\mathbf{r}) = {}^t(S^x(\mathbf{r}), S^y(\mathbf{r}), S^z(\mathbf{r}))$ is a spin-1/2 operator at a lattice site \mathbf{r} and h_ℓ is a local hamiltonian which depends on several spins at $\mathbf{r}_1, \mathbf{r}_2, \dots$. It generically breaks several symmetries explicitly such as a parity, a chiral symmetry, and a time reversal symmetry. The operator T_μ is a translation in μ -direction, $T_\mu \mathbf{S}(\mathbf{r}) T_\mu^\dagger = \mathbf{S}(\mathbf{r} + \mathbf{a}_\mu)$ (\mathbf{a}_μ is a unit translation in μ direction). We use a periodic boundary condition $T_\mu^{L_\mu} = 1$ ($m_\mu = 0, \dots, d$) to avoid disturbing bulk properties by possible edge states. *We propose to use twisted boundary conditions for the spin model and take the twists as the parameters x as discussed below.*

Local Gauge Transformation and Twists : Let us consider a local gauge transformation of a string type, that is, local spin rotations at a unit cell label \mathbf{m} as $\mathbf{S}'_\theta(\mathbf{r}_\eta^\mathbf{m}) = \mathbf{Q}(\gamma) \mathbf{S}(\mathbf{r}_\eta^\mathbf{m})$ with 3×3 matrix $\mathbf{Q}(\gamma) = e^\gamma \mathbf{X}$, $\gamma = \mathbf{m} \cdot \boldsymbol{\theta}$ where $X^{\alpha\beta} = \frac{1}{2} i n^\gamma \text{Tr } \sigma^\alpha \sigma^\beta \sigma^\gamma$, $\boldsymbol{\theta} = (\theta_1, \dots, \theta_d)$ and $\mathbf{n} = (n_x, n_y, n_z)$ ($|\mathbf{n}| = 1$) is a fixed rotation axis. Also η is a label to distinguish intra unit cell spins. The simplest example is given by taking $\mathbf{n} = (0, 0, 1)$

as $\mathbf{Q}^z(\gamma) = \begin{pmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$ with $\gamma = \mathbf{m} \cdot \boldsymbol{\theta}$. We further assume the local hamiltonian h_ℓ is of the gauge interaction type as

$$\begin{aligned} h_\ell(\mathbf{S}(\mathbf{r}_1), \mathbf{S}(\mathbf{r}_2), \dots) &= h^G(\boldsymbol{\theta} = \mathbf{0}; \{\mathbf{r}_i - \mathbf{r}_j\}; \mathbf{S}(\mathbf{r}_1), \mathbf{S}(\mathbf{r}_2), \dots) \\ &= h^G(\boldsymbol{\theta}; \{\mathbf{r}_i - \mathbf{r}_j\}; \mathbf{S}'_\theta(\mathbf{r}_1), \mathbf{S}'_\theta(\mathbf{r}_2), \dots) \\ &\equiv h_\ell^\theta(\mathbf{S}'_\theta(\mathbf{r}_1), \mathbf{S}'_\theta(\mathbf{r}_2), \dots) \end{aligned}$$

with some function h^G . That is, *the twisting parameters only affect the hamiltonian through the relative positions of the local spins*. Examples of such interactions for the above rotation around z -axis are $h_\ell^{\text{pair}} = {}^t \mathbf{S}(\mathbf{r}_1) \mathbf{J} \mathbf{S}(\mathbf{r}_2)$ with $\mathbf{J} = J \text{diag}(1, 1, \lambda)$ and $h_\ell^{\text{sb}} = J_c \mathbf{S}(\mathbf{r}_1) \cdot (\mathbf{S}(\mathbf{r}_2) \times \mathbf{S}(\mathbf{r}_3)) = J_c \epsilon_{ijk} \mathbf{S}_i(\mathbf{r}_1) \mathbf{S}_j(\mathbf{r}_2) \mathbf{S}_k(\mathbf{r}_3)$ [34]. They transform respectively as $h^{\text{pair}} = \frac{J}{2} (e^{-i(\theta_1 - \theta_2)} S_{1\theta_1}^+ S_{2\theta_2}^- + \text{h.c.}) + \lambda S_{1\theta_1}^z S_{2\theta_2}^z$, $h^{\text{sb}} = \frac{J_c}{2} S_{1\theta_1}^z (ie^{-i(\theta_2 - \theta_3)} S_{2\theta_2}^+ S_{3\theta_3}^- + \text{h.c.}) + (\text{cyclic perm.})$, $\theta_i = \mathbf{m}_i \cdot \boldsymbol{\theta}$, $i = 1, 2, 3$ where \mathbf{m}_i is a unit cell labeling of the spin $\mathbf{S}(\mathbf{r}_i)$.

The hamiltonian H^P is periodic in the original representation by \mathbf{S} 's but is not periodic in the one by twisted \mathbf{S}_θ 's as $\mathbf{S}'(T^{L_\mu} \mathbf{r}) = T'^{L_\mu} \mathbf{S}'(\mathbf{r})$ with $T'^{L_\mu} = \exp(-\hat{n}_\mu \theta_\mu L_\mu \mathbf{X})$.

Now let us define a translational invariant twisted hamiltonians H^T by a representation by the twisted \mathbf{S}'_θ as $H^T(\boldsymbol{\theta}) = \sum_{\mathbf{m}} T'^{\mathbf{m}} h_\ell^\theta(\mathbf{S}'_\theta(\mathbf{r}_1), \mathbf{S}'_\theta(\mathbf{r}_2), \dots) T'^{\mathbf{m}^\dagger}$ with a periodic boundary condition $T'^{L_\mu} = 1$. In the original spin operators \mathbf{S} , H^T is given by H^P with the twisted boundary condition $T_\mu^{L_\mu} = \exp(+\theta_\mu L_\mu \mathbf{X})$.

The two hamiltonians, H^P and H^T , are both translationally invariant in representations by \mathbf{S} and \mathbf{S}'_θ respectively. One may expect an macroscopic $\mathcal{O}(V)$ energy difference between their ground state energies. However, as discussed, the contribution should be at most $\mathcal{O}(|\partial_\mu V|)$ due to the gauge invariance where $|\partial_\mu V|$ is a (hyper) area of the system perpendicular to the r_μ -axis where $V = L_1 \cdots L_d$. That is, the difference of the energy should be a finite size effect. Thus the difference between H^P and H^T is negligible in the thermodynamic limit $V \rightarrow \infty$ when we discuss the bulk properties in a usual manner.

Another important point for the present construction is that the twisted hamiltonian H^T is translational invariant in the \mathbf{S}_θ representation. Then edge states never appear in any representation, which is especially important to pick up only bulk properties through probes by twisted boundary conditions.

Degeneracies and Ground State Multiplet : A topological order on a non-zero genus Riemann surface is one of the reasons for the ground state degeneracy, which is the topological degeneracy[11]. The simplest example is just a manybody state with two-dimensional periodic boundary conditions[31, 32]. Also if the system has a standard symmetry breaking, such as ising orders, a fi-

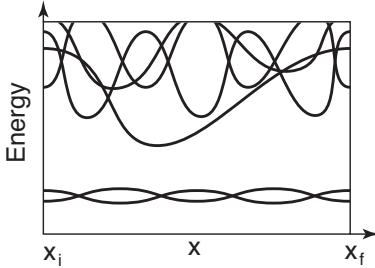


FIG. 1: Schematic spectral flow with parameters x .

nite system has almost degenerate ground states corresponding to linear combinations of the symmetry broken states[35]. For a finite system, the degeneracy can be lifted and the splitting is estimated as $\approx e^{-CV}$ for the symmetry broken states. Also if the ground state has a finite spin moment which may not be macro as a ferromagnet, there occurs a spin degeneracy. Some of these degeneracies can be approximate for a finite system and may be sensitive to the boundary condition and twisting parameters, such as θ_μ 's. In these cases, the lowest energy gap is not a physical one and may vanish in the thermodynamic limit. The physical energy gap for the bulk is an energy gap above these almost degenerate states. We define a ground state multiplet by a collection of these almost degenerate states near the ground state and define a Chern number for this ground state multiplet. (See the Fig.1) [36] Since the two hamiltonians H^P and $H^T(\boldsymbol{\theta})$ differ only boundary terms, bulk properties of the two should be the same. Then, for the topological insulators, the energy gap above the ground state multiplet is stable against perturbations. If the ground state multiplet is well separated from the above in a finite system, *we do not need to take the thermodynamic limit*.

The twist we proposing is a boundary perturbation in a particular representation. However it also preserve the translational symmetry up to a unitary equivalence. Then, based on a discussion of edge state picture, we expect an energy separation of the topological degeneracy, that is, a band width of the multiplet by the twist as $e^{-L/\xi}$ where L is a minimum linear dimension of the system and ξ is a typical length scale of the ground state multiplet. It can be different from the conventional broken symmetric cases.

Chern Numbers for the Spins : Let us define a total parameter space by $\mathcal{V} = \{(\theta_1, \dots, \theta_d) | \theta_\mu \in [0, 2\pi/L_\mu]\}$. Since $\exp(2\pi\mathbf{X}) = \mathbf{I}_3$, we have $H^T(\boldsymbol{\theta} + (\dots, 0, \theta_\mu + 2\pi/L_\mu, 0, \dots)) = H^T(\boldsymbol{\theta})$ in the \mathbf{S} -representation. Then the twisted hamiltonian $H^T(\boldsymbol{\theta})$ is well defined on \mathcal{V} without boundaries as $\mathcal{V} = T^d$. [37] Any two dimensional integration surface $\mathcal{S} (\subset \mathcal{V})$ without boundaries is used to define the Chern numbers. $\mathcal{S} = T_{ij}^2 = \{(\theta_i, \theta_j)\}$ is the simplest example.

Now define a ground state multiplet $\Psi(x), x \in \mathcal{V}$. It is a $N \times q$ matrix as $\Psi(x) = (\psi_1(x), \dots, \psi_q(x))$ with $H^T(x)\psi_j(x) = \epsilon_j\psi_j(x), j = 1, 2, \dots, \epsilon_i \leq \epsilon_j, (i < j)$, where ψ_j is a column vector in a many spin Hilbert space with a dimension N and q is a dimension of the ground state multiplet. The *generic energy gap condition* for the multiplet is given as $\epsilon_q(x) < \epsilon_{q+1}(x), \forall x \in \mathcal{S}$. This is a definition of the topological insulators.

Define a non-Abelian connection one-form \mathbf{A} which is an $q \times q$ matrix as $\mathbf{A} = \Psi^\dagger d\Psi$ and a field strength two-form $\mathcal{F} = d\mathbf{A} + \mathbf{A}^2$. The first Chern number[2] is then defined by $C_S = \frac{1}{2\pi i} \int_S \text{Tr } \mathcal{F} = \frac{1}{2\pi i} \int_S \text{Tr } d\mathbf{A}$. It is a topological integer which is stable against perturbation unless the generic gap collapses. We use these integers depending on a choice of \mathcal{S} to characterize the topological orders. Changing a basis within the multiplet space, $\Psi'(x) = \Psi(x)\omega(x)$, ($\omega\omega^\dagger = \mathbf{I}_q$) gives a gauge transformation $\mathbf{A}' = \Psi'd\Psi' = \omega^{-1}\mathbf{A}\omega + \omega^{-1}d\omega$ and $\mathcal{F}' = \omega^{-1}\mathcal{F}\omega$ [4, 28]. The Chern number is a gauge invariant but we need to fix the gauge to evaluate this expression[28]. Take a generic arbitrary multiplet, Φ , and define an overlap matrix as $\mathbf{O}_\Phi = \Phi^\dagger P\Phi$ where $P = \Psi\Psi^\dagger$ is a projection into the ground state multiplet which is a gauge invariant. Then define regions $\mathcal{S}_R^\Phi, R = 1, 2, \dots$, as (infinitesimally) small neighborhoods of zeros of $\det \mathbf{O}_\Phi(x)$ and \mathcal{S}_0^Φ as a rest of \mathcal{S} . Then the first Chern number is written as $C_S = -N_\Omega^T(\mathcal{S}) = -\sum_{R \geq 1} n_\Omega^R(\mathcal{S}_R^\Phi), n_\Omega^R(\mathcal{S}_R^\Phi) = \frac{1}{2\pi} \oint_{\partial\mathcal{S}_R^\Phi} d'\Omega$.

The field Ω is defined as $\Omega(\tilde{\Phi}, \Phi) = \text{Arg det } \tilde{\Phi}^\dagger P\Phi = \text{Arg det } \eta - \text{Arg det } \tilde{\eta}$ where $\tilde{\Phi}$ is also another generic arbitrary multiplet, $\eta = \Psi^\dagger\Phi$ and $\tilde{\eta} = \Psi^\dagger\tilde{\Phi}$. The matrices η and $\tilde{\eta}$ depend on the choice of the multiplet Ψ but the difference of the arguments is a gauge invariant.

The field Ω depends on a choice of Φ and $\tilde{\Phi}$ but the total vorticity $N_\Omega^T(\mathcal{S})$ is a gauge invariant and independent of the choice. *The field Ω reflects a phase sensitivity of the multiplet by the twist* when one fixes Φ and $\tilde{\Phi}$. It is illustrative to show Ω and it supplies information of the ground state multiplet. Also when the integration surface \mathcal{S} is contractible to a point keeping a generic energy gap, the Chern number vanishes from a topological stability.

Ex.1:Two-Dimensional Spin Model : The present formulation can be effective for characterization of topological ordered phases in any dimensions, such as chiral spin states[34]. *To have a finite Chern number, one needs to break time reversal symmetry* as for the quantum Hall states [38]. The simplest example of h_ℓ can be a sum of local pair-spin interactions h_ℓ^{pair} with a symmetry breaking term h_ℓ^{sb} discussed above as $h_\ell = \sum_{\text{pair}} h_\ell^{\text{pair}} + h_\ell^{\text{sb}}$. Here let us just show an example with a degeneracy to show the present general procedure. Considering only a nearest neighbor exchange interaction and assume $\mathbf{n} = (0, 0, 1)$, the local hamiltonian is given as $h_\ell^\theta = \sum_{\mu=x,y} J \left(\frac{1}{2} (e^{-i\theta^\mu} S_{\theta+}^\mu S_{\theta-} + e^{i\theta^\mu} S_{\theta-}^\mu S_{\theta+}) \right)$

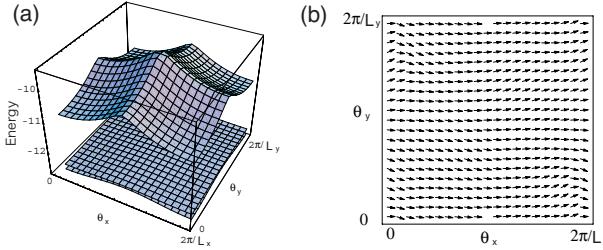


FIG. 2: (a)Three lowest energies of the XXZ model on a 4×4 square lattice with twists in the total $S_z = 0$ sector is shown. ($\lambda = 1.3$) (b) A field Ω of the ground state multiplet composed of the lowest two eigen states for some choice of $\Phi, \tilde{\Phi}$.

$\lambda S_{\theta z}^{\mu} S_{\theta z}$) where $S_{\theta}^{\mu} = S_{\theta}(T^{\mu} \mathbf{r})$ and $S_{\theta} = S_{\theta}(\mathbf{r})$. In the case, the twisted boundary condition for $H^T(\theta)$ in \mathcal{S} is given by the following matrix $T_{\mu}^{L_{\mu}} = Q^z(\gamma)$ with $\gamma = \theta_x L_x + \theta_y L_y$. Then we can take a 2 dimensional torus $T^2 = \{(\theta_x, \theta_y) | 0 \leq \theta_{\mu} \leq 2\pi/L_{\mu}\}$ for the integration surface \mathcal{S} . This is a nearest neighbor XXZ model on a square lattice with twists. With an ising anisotropy, $\lambda > 1$, the ground state of an infinite system has a long range order and has a finite energy gap. We show numerical results for a system with $J = 1$ and $\lambda = 1.3$. The ground state of a finite size system is given by a bonding state between two symmetry broken states with antiferromagnetic (ising) order. The next lowest state is an anti-bonding state of them and the energy separation between is expected to be $\propto e^{-L_x L_y / \xi^2}$ where ξ is a typical length scale. A physical ising gap to flip one ordered spin is given the one above, that is, the second lowest one. Therefore the ground state multiplet is composed of the two low lying states including the finite size ground state. (See Fig.2(a)) The field Ω of the two dimensional ground state multiplet is shown in Fig.2(b). As discussed in the reference[28], the Chern number is a sum of the vorticity at the zeros of $\det \mathcal{O}_{\Phi} = |\det \boldsymbol{\eta}|^2$. In the present example, it is 0 as expected for a chiral symmetric system.

Ex.2, Manyparticle States in the First Quantized Form : The same procedure is also applied for a manyparticle state in the first quantized form, such as the generic FQH States $\Psi_k(x; \mathbf{r}_1, \sigma_1; \dots; \mathbf{r}_N, \sigma_N)$ where k denotes a label of the (topological) degeneracy of the ground state multiplet and $x = (\theta_x, \theta_y)$ is a set of parameters specifying twisted boundary conditions on a torus[32]. By taking a reference multiplet as $\Phi_{\xi}(\mathbf{r}_1, \sigma_1; \dots; \mathbf{r}_N, \sigma_N) = \delta_{\sigma_1 \sigma_1^{\xi}} \delta(\mathbf{r}_1 - \mathbf{r}_1^{\xi}) \dots \delta_{\sigma_N \sigma_N^{\xi}} \delta(\mathbf{r}_N - \mathbf{r}_N^{\xi})$, $\xi = 1, \dots, q$. The Chern number for the degenerate multiplet is given by the field $\Omega(x) = \text{Arg} \det \tilde{\boldsymbol{\eta}}^{\dagger} \boldsymbol{\eta}$ with $\{\boldsymbol{\eta}\}_{\xi k} = \Psi_k(x; \mathbf{r}_1^{\xi}, \sigma_1^{\xi}; \dots; \mathbf{r}_N^{\xi}, \sigma_N^{\xi})$ and $\{\tilde{\boldsymbol{\eta}}\}_{\xi k} = \Psi_k(x; \mathbf{r}_1^{\tilde{\xi}}, \sigma_1^{\tilde{\xi}}; \dots; \mathbf{r}_N^{\tilde{\xi}}, \sigma_N^{\tilde{\xi}})$ where $k, \xi, \tilde{\xi}$ run over $\{1, \dots, q\}$. The Chern number is evaluated as a total

vorticity of Ω at the zeros of $|\det \boldsymbol{\eta}|^2$ [28].

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- [35] Y. Hatsugai, Phys. Rev. B **56**, 12183 (1997).
- [36] Since the hamiltonian $H^T(\theta)$ is translationally invariant, $[H^T, T'_\mu] = 0$. That is $T'_\mu = e^{ik_\mu}$ with $k_\mu = 2\pi m_\mu/L_\mu$, $m_\mu = 0, \pm 1, \pm 2, \dots$, the ground state multiplet may compose of states with different k_μ . We may define the Chern numbers using these conserved quantum numbers. However it is natural to discuss (almost) degenerate states as a ground state multiplet[28].
- [37] When we use a representation by \mathcal{S}_θ , $H^T(\theta + (\dots, 0, \theta_\mu + 2\pi/L_\mu, 0, \dots)) \neq H^T(\theta)$ and it is not well defined on the surface \mathcal{S} . It is just well defined up to an unitary equivalence.
- [38] Non-trivial examples with finite Chern numbers for spin models are under studies in collaboration with X.-G. Wen. (unpublished)